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Statement of Work

The purpose of this program is to compile and critically evaluate diffusivity and viscosity data on gas, liquid, solid and turbulent flow systems. The program has been in operation for eighteen months. Progress in the various areas of the program is discussed separately in the following sections.

I. Diffusion in Gases

The evaluation of gaseous diffusion measurements for binary noble gas mixtures is almost complete. It appears that diffusion coefficients may be reasonably well correlated from 273 to 10,000 °K. Measurements at low temperatures for the noble gases are scarce. Diffusion measurements for other substances have been indexed according to gas pair and the data values are being added to "system" reference cards.

Most noble gas-pair diffusion data have been least-squared according to the equation $D = D_0 T^S$. Weights were assigned to each measurement; all radon containing systems were weighted zero. The calculations are presently being checked. At elevated temperatures, say $T > 1000^\circ\text{K}$, diffusion coefficients were calculated based on two independent measurements of molecular beam scattering (MIT - Amdur, et al. and USSR - Leonas et al). An inverse-power repulsion potential model was assumed to calculate collision integrals. These results are in excellent agreement with each other and data at lower temperatures. Beam results are being extended to lower temperatures over which direct measurements exist. An interpolation function assumed was an exponential potential. Monchick (1959) tabulated values of the collision integrals for the exponential intermolecular force potential.

These values plus the parameters assigned by Amdur and Mason (1958) were used to calculate diffusion coefficients. For the He-Ar system calculated results and direct measurements are consistent to within a few per cent.

To augment the available self-diffusion coefficient measurements of the noble gases, viscosity data will be used to calculate D_{11} values over the maximum possible temperatures range. The data for noble gas unlike mixtures will be finalized and evaluation and compilation of other gaseous diffusion measurements will be initiated.

II. Liquid Phase Molecular Transport Coefficients

The program of compiling and evaluating molecular transport coefficients (diffusivity and viscosity) in liquid phase systems has proceeded to a point where concurrent attention is being devoted to a comprehensive cataloguing and information retrieval system along with the continuing tasks of literature search and data evaluation.

The last Annual Report presented some preliminary findings on experimental techniques and correlation methods that have been used for 56 different liquid-liquid systems representing eight different solvents, 47 compounds and elements in water, and for three amine compounds in benzene; all of the data being for the experimental condition approaching infinite dilution. During the current report period, attention has been centered on the compilation of data (diffusivity) in which the solution composition has been a prime variable. With this compilation, most of the data on the molecular diffusion coefficient on systems in Class I (Polar Solvents with Ionizing or Non-Ionizing Solutes) and Class II (Non-Polar Solvents with Ionizing or Non-Ionizing Solutes) will have been completed for most of the readily available data up through 1966. Class III (Inorganic and Liquid Metal Solvents with Organic or Inorganic Solutes) compounds are being deferred for the time being, insofar as comprehensive coverage is concerned, until the above compilations are complete and the information cataloguing and retrieval systems is perfected.

The initial companion work on viscosities is just now getting underway, and initial efforts are being directed to those systems for which diffusion data are being evaluated, and then large scale coverage of viscosity information for all systems will follow with the major stress being placed on binary systems.

The information retrieval system is being based on all information being catalogued on data processing cards and/or tapes and with a coding system to permit retrieval of data according to a wide variety of planned programs. To afford a better insight into the parameters necessary for coding and recall, a survey has been completed on all the various correlating theories and schemes that have been proposed for correlating or predicting molecular diffusion coefficients for liquids...either for infinitely dilute conditions or concentrated solutions...these will be a help in planning the retrieval programs as well as assisting in the data evaluation.

III. Diffusion in Inorganic Solids

During the past six months our work has been involved primarily with the study of self-diffusion in the alkali halides. All of the literature data have been reviewed and collated. These data are now being correlated and plotted. Least squares curve fitting using the OMNITAB computer program is being used to reduce the data to numerical form and to place confidence limits on the pre-exponential and activation energy terms in the equations.

Some of the problems regarding the reported diffusion coefficient for Ag in AgCl have been further reviewed and studied. In examining the original data upon which the Compton & Maurer work (J. Phys. Chem. Solids 1, 191) was based we find that the equation suggested do not fit the data. We have fitted the original data using a two segment curve and the OMNITAB least squares fitting computer program. The conductivity data was similarly fitted using the Einstein equation for converting to diffusivity. Both the equations for diffusivity and for conductivity reported in the

previous compilation presented in the American Institute of Physics handbook are definitely in error. The interstitially diffusion mechanism is now supported and the data of Reade & Martin (J. Appl. Physics 31, 1965) are in much closer agreement with the Compton and Maurer data than they were with the equation erroneously reported in the literature.

IV. Diffusion in Polymer-Diluent Systems

The major portion of our effort since the last report has been spent in collecting and cataloguing the various articles located in our literature search. The literature search continues but is now concerned mainly with filling in some of the gaps and with current articles. We feel that we now have in our files the principal articles published through 1966.

Most of the articles in our possession have been catalogued and an index file prepared which lists diffusion medium, diffusing substance and the physical nature of the diffusing substance for each polymer-diluent system evaluated in each articles. We plan to use this file to develop a tabulation of data for each of the systems of interest. This portion of the program is just starting and should be completed by the fall. Evaluation of data will be made at the same time that the data for each system is tabulated. Only diffusivity data is to be evaluated at this time with an analysis of the use of our large collection of permeation rate data to determine diffusivities deferred until later.

V. Turbulent Transport Coefficients

Research on turbulent transport phenomena is being actively pursued at a number of laboratories. In nearly every case the work is directed toward a rather narrow and specific goal and deals with limited ranges in properties and geometry of the systems being studied. To provide us with a better understanding of the in-house NASA work visits were made to three laboratories during this re-

porting period. These were:

NASA - Langely On December 15, 1966 Mr. Ivan E. Beckwith arranged the visit. Dr. Marchello gave a one hour presentation to 21 NASA personnel. It was followed by about another hour of group discussion. The remainder of the day was spent in conferences with interested individuals. Results of the project will be of direct value, particularly in their work on supersonic boundary layers and combustion.

NASA - Houston On February 21, 1967 Mr. Robert C. Reid arranged the visit. Through earlier telephone conversations it was established that the results of the project would have a secondary influence on their work. Dr. Marchello discussed the project over an extended luncheon with seven NASA personee.

NASA - Huntsville On April 14, 1967 Mr. W. D. Murphree arranged the visit. Dr. Marchello gave a one hour presentation to 28 NASA personnel. It was followed by six presentations of work at Huntsville. The remainder of the day was spent in conferences with interested individuals. Results of the project will be of direct value in their work, particularly on free shear layers, exhaust plumes, surface pressure fluctuations and turbulence in liquids.

The project is progressing well. The major portion of our effort since the last report has been spent in collecting and cataloguing the material located in the literature survey. The compilation and evaluation work will represent a major portion of our effort during the next period.

VI. Personnel

The investigation of diffusion in gases is directed by Dr. E. A. Mason. He is assisted by two graduate students, Mr. T. R. Marrero and Mr. Kenneth Himmelstein.

The liquid diffusion survey is directed by Dr. R. B. Beckmann, with the assistance of two graduate students, Mr. D. J. Hancis and Mr. P. N. Vashist and a part-time research associate Mrs. M. C. Bailey.

The investigation of diffusion in inorganic solids is directed by Dr. L. P. Skolnick. He is assisted by one graduate student, Mr. Patrick Sung.

The polymer diffusion survey is directed by Dr. T. G. Smith, with the assistance of a graduate student, Mr. Ronald Heck.

Dr. J. M. Marchello is directing the turbulent transport survey and is assisted by one graduate student, Mr. E. F. Logan.